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November 12, 2007

Engineering Fracture Mechanics

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The Cohesive Continuum Framework for Analysis of Fracture in Solid Bodies

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Abstract

Embedding cohesive surfaces into finite element analysis is a widely used technique for the numerical simulation of material separation (i.e., crack propagation). Typically, a traction-separation law is used which relates the magnitude of the cohesive traction to the distance between the separating surfaces. Thus the characterization of fracture in such models is decoupled from the bulk constitutive response, as well as containing no intrinsic dependence on material stretching in the plane of the fracture surface. In this work, the "Cohesive Continuum Framework" (CCF) is presented as a further development of the cohesive zone idea, wherein the traction-separation law – and therefore the fracture phenomenology – derives directly from the bulk constitutive law. The immediate goal is an improved modeling framework for ductile fracture in metals wherein 3D effects such as crack-top triaxiality can play a significant role in fracture behavior. The CCF is implemented in an explicit 3-dimensional finite element code. Proof-of-concept analyses using both linear elastic and Gurson void growth constitutive relations are presented. A 3-point bend simulation is found to give good agreement with experimental results.

Keywords: cohesive continuum, cohesive zone, ductile fracture, finite elements

1. INTRODUCTION

Cohesive zone (CZ) modeling is now a well-established approach in computational fracture mechanics. The central element of the CZ concept is a rule which associates a traction vector with a

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prescribed separation-displacement history. This rule is applied pointwise on a surface pair that is in the process of separating, such that the separation is resisted by opposing tractions. In this modeling paradigm, the traction-separation rule is dependent on the material, and is properly regarded as part of the material's constitutive description, alongside the bulk constitutive law.

Traction-separation rules can generally be categorized as either initially elastic or initially rigid. In the case of initially elastic cohesive laws, such as those presented by Needleman [3,4], Rice and Wang [5], Xu and Needleman [6-8], and Tvergaard and Hutchinson [9] among others, the closing traction is initially zero at zero separation. Thereafter, the traction increases with increasing separation until a maximum value is reached, after which the traction diminishes to zero at some finite relative displacement. In contrast, the initially rigid class of cohesive laws [10-12] proposes that the prospective separation surfaces remain connected until a critical traction is reached, whereupon the traction decreases continuously to zero as separation proceeds. In both cases, post-peak unload/reload behavior is generally assumed to occur along a straight trajectory from the origin; i.e. the cohesive rule is assumed to be irreversible.

The compliance introduced by initially elastic cohesive laws is unphysical, but is generally of little consequence in finite element calculations where only a single pre-existing surface is designated as the fracture surface. This is appropriate for highly symmetric scenarios, where the crack path can be inferred from symmetry. However, if ubiquitous pre-existing cohesive surfaces are specified, e.g. at all inter-element facets [10, 12], then the cohesive compliance introduces a mesh dependence which ultimately culminates in zero stiffness of the body as the mesh is refined continuously. Klein et al. [13] provide a thorough discussion of this issue and suggest guidelines to mitigate its effects.

Initially rigid cohesive laws are free of the unphysical mesh dependence exhibited by initially elastic laws, but come with their own set of complications. For example, in dynamic finite element calculations, if a cohesive element is unloaded immediately after its critical traction is first reached, then the unload-reload response of the element can exhibit arbitrarily high stiffness. This

circumstance presents difficulties in relation to explicit time integration of the equations of motion. A more basic issue is that of time-continuity of the nodal cohesive forces across the separation event. As discussed by Papoulia et al. [14], time continuity of these forces emerges as an important issue in the post-peak behavior of the separating surfaces, due to the negative slope of the traction-separation rule. Unless special care is taken, the nodal cohesive forces suffer a discontinuity as the critical traction is reached, causing a shock-type loading at the surface pair. In view of the negative-stiffness cohesive law, this shock can drive the system dynamics in such a way that the cohesive forces degrade prematurely, and in a physically unrealistic manner. Papoulia et al. [14] propose an initially rigid formulation that enforces time continuity through a procedure that modifies the cohesive tractions at initiation. However, this formulation suffers from traction locking, for which no remedy is immediately apparent.

By way of introduction of the developments proposed herein, two fundamental features of the conventional CZ approach bear particular emphasis. First, the CZ traction-separation rule applies to *a pair of surfaces that are in the process of separating*. It cannot, by itself, explicitly provide for a *transition* from smoothly-deforming internal material surface to separating surface pair. The second feature of particular relevance here is that the traction-separation rule is the subject of a separate constitutive postulate that is unrelated to the bulk stress-strain behavior. The latter controls the mechanical response of material points up until the instant that separation initiates, after which the completely unrelated traction-separation rule takes over. It might be said that the standard CZ approach attempts to model fracture by describing what happens to material surfaces only after they have begun to separate, and not by delineating the conditions under which the transition to separation takes place. The approach of Oliver et al. [33,34], on the other hand, attempts to address this disconnect by extracting the cohesive law from the softening branch of the bulk constitutive law, using strong-discontinuity kinematics.

It is asserted that the two above-described features of the classical CZ approach engender serious limitations with respect to physically realistic modeling of fracture. The theoretical

approach proposed herein, called the *Cohesive Continuum* framework, represents an attempt to address these limitations by connecting, in a natural way, the traction-separation behavior with the bulk constitutive law. A particular goal of this approach is construction of cohesive laws that reflect a physically meaningful relationship between the fracture behavior on the one hand, and three-dimensional aspects of the near-tip fields, such as stress triaxiality, on the other. In this way, the physically observed influence of hydrostatic stress in the near-tip region can be modeled in a controllable manner. In this connection, it is mentioned that Siegmund and Brocks [17, 18], remaining within the conventional CZ format, present a model in which the cohesive law is modified by the stress triaxiality in the adjacent bulk material. Their motivation is largely the same as for the present work: to consider the state within the bulk continuum when simulating material separation.

The Cohesive Continuum framework is introduced in the next section. This approach differs from standard cohesive-zone methods in that it seeks to specify cohesive stresses, separately-postulated two-dimensional relationship, but instead from the complete 3-dimensional constitutive response. This is accomplished through specification of a deformation-gradient-like kinematic tensor that involves components of the bulk deformation gradient, the opening displacement, and a length scale. This kinematic measure is used to drive the bulk constitutive response. The resulting material stress state is, in turn, applied to the body in a manner that supplies cohesive closing tractions in the rupture zone.

2. THE COHESIVE CONTINUUM FRAMEWORK

Kinematics

Consider a material body that occupies an open spatial region B , with boundary surface ∂B at time (t) . The body also occupies the open region B_0 , with boundary surface ∂B_0 , at some reference time prior to any surface separation. Let the position of a typical material point be $\mathbf{x} \in B$ and $\mathbf{X} \in B_0$ in the current and reference configurations respectively. Now consider a smooth, but otherwise arbitrary surface $\Gamma_0 \subset B_0$ with unit normal \mathbf{N} and tangent unit vectors \mathbf{M}_α ($\alpha=1, 2$) such that $\{\mathbf{N}, \mathbf{M}_1, \mathbf{M}_2\}$

forms a right-handed orthonormal triad at every point on Γ_0 . The surface Γ_0 will be called the *rupture surface*, as it is the surface that ultimately separates into a pair of new boundary surfaces. For any point $\mathbf{X} \in \Gamma_0$, there exists an open neighborhood $R \subset B_0$ of \mathbf{X} such that $R = R^+ \cup R^- \cup (R \cap \Gamma_0)$ where $R^+ \cap R^- = \emptyset$; i.e. the surface Γ_0 divides the region R into two disjoint open regions $R^{+,-}$. The surfaces $(\bigcup_{\mathbf{X} \in \Gamma_0} R^{+,-} \mid \Gamma_0)$ are referred to as $\Gamma_0^{+,-}$ respectively. Whereas $\Gamma_0^{+,-}$ are geometrically identical to Γ_0 , their respective outward unit normal vectors $\mathbf{N}^{+,-}$ satisfy $\mathbf{N}^+ + \mathbf{N}^- = \mathbf{0}$. The current position vector and surface deformation gradients on $\mathbf{X} \in \Gamma_0^{+,-}$ are defined as:

$$\mathbf{x}^{+,-} = \lim_{\xi \rightarrow 0^+} \mathbf{x}(\mathbf{X} - \xi \mathbf{N}^{+,-}), \quad (1)$$

$$\mathbf{F}^{+,-} = \lim_{\xi \rightarrow 0^+} \mathbf{F}|_{\mathbf{X} - \xi \mathbf{N}^{+,-}}. \quad (2)$$

Further, we define the *gap vector* on Γ_0 as:

$$\mathbf{v} = \mathbf{x}^+ - \mathbf{x}^-, \mathbf{X} \in \Gamma_0. \quad (3)$$

Now consider a pair of surfaces $\partial\Lambda_0^{+,-}$, such that they are a distance $\lambda/2$ from Γ along the normal $\mathbf{N}^{+,-}$. The surfaces $\partial\Lambda_0^{+,-}$ can be said to bound a material layer Λ_0 of thickness λ as shown in Figure 2. The role of Λ_0 is to specify a region of material that is actively undergoing rupture, and is therefore subject to special treatment.

Throughout the solution of a continuum boundary value problem, the deformation gradient \mathbf{F} and its history may be used to generate kinematic “inputs” to the constitutive law. As in the continuum problem, the Cohesive Continuum Framework relies on a local constitutive evaluation everywhere in the body B . However, the CCF seeks to distribute the effects of a discontinuity (i.e., non-zero gap vector) across the layer Λ . Thus the standard deformation gradient is replaced by a modified gradient-like kinematic tensor (\mathbf{G}) within Λ . This tensor, which is used to define a material state that is useful for the purpose of assessing progression towards separation, is defined as:

$$\mathbf{G} = \begin{cases} \mathbf{F} + \frac{1}{\lambda} \mathbf{v} \otimes \mathbf{N} & \mathbf{X} \in \Lambda_0 \\ \mathbf{F} & \mathbf{X} \notin \Lambda_0 \end{cases} . \quad (4)$$

Equation (4) states that the \mathbf{G} is equal to the bulk deformation gradient \mathbf{F} , plus an additional term that is proportional to the gap vector (\mathbf{v}) as defined in Equation (3). To illustrate the ramifications of this definition, it is useful to examine how \mathbf{G} transforms a material line element lying along the direction \mathbf{a}_0 in the reference configuration. The component of \mathbf{a}_0 that lies in the direction of \mathbf{N} is transformed by the deformation gradient \mathbf{F} , plus the length-scale-normalized gap vector, i.e.

$\mathbf{GN} = \mathbf{FN} + \frac{\mathbf{v}}{\lambda}$. In contrast, the components of \mathbf{a}_0 that lie in the plane of Γ_0 ($\mathbf{M}_1, \mathbf{M}_2$) are

transformed by \mathbf{F} only, and thus are unaffected by the gap vector.

Rupture Function

A *material rupture function* $\Phi(Q, \mathbf{X}, \mathbf{K})$ is defined to provide a quantitative measure of the progression towards rupture at a material point and in a particular direction. The function's arguments consist of the material state Q , the reference position vector \mathbf{X} , and a unit vector \mathbf{K} . A pair of critical values $\Phi_1(\mathbf{X})$ and $\Phi_2(\mathbf{X})$ are defined throughout the body as the values of $\Phi(Q, \mathbf{X}, \mathbf{K})$ at which the rupture process initiates and completes, respectively. If $\Phi < \Phi_1 \quad \forall \mathbf{X} \in B_0$ and for all \mathbf{K} , then no rupture is indicated, and the standard continuum theory applies to the entire body B_0 . If there exists some material point $\mathbf{X} \in B_0$ where $\Phi_1 < \max_{\mathbf{K}} \Phi(Q, \mathbf{X}, \mathbf{K}) < \Phi_2$, then there exists a rupture surface Γ_0 at \mathbf{X} with unit normal \mathbf{N} , where \mathbf{N} is the \mathbf{K} which maximizes $\Phi(Q, \mathbf{X}, \mathbf{K})$. Thus the path of the surface-separation front is determined by the value of \mathbf{K} that maximizes Φ . For any material point at which $\Phi(\mathbf{X}, \mathbf{N}, Q) = \Phi_2$, the surfaces $\Gamma_0^{+,-} \in \partial B_0$, and are thereafter subject to external boundary conditions. Also of note is the inclusion of the position vector \mathbf{X} in Φ, Φ_1 , and Φ_2 , which allows for material heterogeneity in the rupture behavior. Finally, as a matter of convenience, we define the *separation coefficient* (s) to track the extent of the separation process:

$$s = \begin{cases} 0 & \Phi \leq \Phi_1 \\ \frac{\Phi - \Phi_1}{\Phi_2 - \Phi_1} & \Phi_1 \leq \Phi \leq \Phi_2, \\ 1 & \Phi \geq \Phi_2 \end{cases} \quad (5)$$

where :

$$\dot{s} \geq 0 \quad .$$

The separation coefficient is a monotonically increasing function of Φ that varies linearly between values of zero at $\Phi=\Phi_1$, and unity at $\Phi=\Phi_2$.

In the CCF, the rupture phenomenology is governed by the manner in which Φ depends on the material state Q . Since the rupture function is given no other information other than the material state, position, and an orientation, the bulk constitutive model must provide state descriptors that are suitable for delineating a progression toward rupture. As an example, if a material were known to rupture through void growth and coalescence, the bulk constitutive model should contain some quantitative measure of void size/fraction. Therefore we stress that the choice of bulk constitutive model remains a primary factor in the behavior of any CCF based model of rupture.

Cohesive Stresses

The previous sections provide a means by which to update the state of the material in Λ , as well as a way to quantify the material's progression towards complete rupture. A manner in which the rupturing material influences the equations of motion within the body is now described. Specifically, the stress state in the rupturing material, which will be referred to as the *cohesive stress*, must influence equilibrium of the body in some manner. In conventional cohesive zone models, this occurs via a closing traction applied to the separation surfaces. This closing traction is typically derived from a traction-separation law, which is unrelated to the constitutive relations used to describe the bulk material. In contrast, the CCF provides for a complete and fully three-dimensional material state derived from the bulk constitutive relation. It is from this stress state that the cohesive stresses are derived. To this end, the cohesive stress is expressed as the standard Cauchy Stress (\mathbf{T}) multiplied by a scalar function:

$$\mathbf{T}_c = r(s) \cdot \mathbf{T} \quad (6)$$

The scalar function $r(s)$ is referred to as the *stress-reduction factor*, and is defined as:

$$r(rs) = \begin{cases} 1 & s = 0 \\ f(s) & 0 < s < 1 \\ 0 & s = 1 \end{cases} \quad (7)$$

$$\frac{df(s)}{ds} < 0$$

The appropriateness of a stress-reduction factor is evident when considering the origin of the Cauchy stresses. The material state, and thus the Cauchy stresses, are derived from constitutive relations driven by the enriched kinematics specified in equation (4). While a non-zero value of \mathbf{v} in \mathbf{G} may imply that the material is not fully connected, this implication is lost when \mathbf{G} is used in the same manner as a standard continuum-based gradient to update the material state. No information pertaining to the separation of the material is passed to the constitutive model; therefore the stresses generated by the constitutive model assume that the material is still fully connected. If the constitutive model does not provide a means for a reduction in load-carrying capacity based on its own "damage" parameters, then a method for reducing the stresses applied to the body must be specified outside the scope of the bulk constitutive relation. Accordingly, the stress reduction factor enforces the requirement that the cohesive stress goes to zero as the separation coefficient approaches unity (i.e. full separation).

It is crucial to observe that the cohesive stresses (\mathbf{T}_c) that result from the modified constitutive response in the layer Λ must be applied in a manner that is consistent with the assumed configuration of Λ . Specifically, we state that the cohesive stress (\mathbf{T}_c) is the appropriate measure of stress to represent the state of the material within Λ . It follows that the discontinuity that bisects Λ implies the stresses in Λ^{+-} must be accompanied by cohesive tractions (denoted by Piola tractions \mathbf{p}_c^{+-}) that are applied to the separating surfaces Γ^{+-} .

To determine appropriate values of these cohesive tractions consider a “filament” \mathcal{L} of material lying normal to Γ (i.e. along \mathbf{N}) and described in the reference configuration by an infinitesimal area $dA \subseteq \Gamma$ and $-\frac{\lambda}{2} < Y_3 < \frac{\lambda}{2}$ - i.e., \mathcal{L} spans Λ . Now consider that the filament undergoes separation at its middle, subject to the cohesive tractions, which tend to hold the halves together. The rate of work on \mathcal{L} per unit cross-sectional area in a quasistatic process is:

$$\begin{aligned} \dot{E}_{\mathcal{L}} &= \int_{-\lambda/2}^{0-} \left((P_c)_{ij} \dot{F}_{ij} \right) dY_3 + \int_{0+}^{\lambda/2} \left((P_c)_{ij} \dot{F}_{ij} \right) dY_3 - (p_i^+ \dot{u}_i^+ + p_i^- \dot{u}_i^-) \\ \text{where :} \\ \mathbf{P}_c &= \mathbf{T}_c \mathbf{F}^{-T} \det(\mathbf{F}) \end{aligned} \quad (8)$$

Now assume for a moment that \mathbf{p}^{+-} were arbitrarily set to zero. If this were the case, then equation (8) indicates that the cohesive stress may act as an unphysical energy source resulting in unstable solutions. This may be explained by noting that equation (8) is the energy balance per unit cross-sectional area over Λ if $\mathbf{P}_c = \mathbf{T}$. The fact that \mathbf{P}_c is not necessarily equal to \mathbf{T} leads to the introduction of an energy source.

Now consider a second scenario, in which the filament \mathcal{L} remains intact, but actually deforms with the deformation gradient equal to \mathbf{G} . In this case, the rate of work done on \mathcal{L} per unit area ($\dot{E}_{\mathcal{L}_2}$) in a quasistatic process is:

$$\dot{E}_{\mathcal{L}_2} = \int_{-\lambda/2}^{\lambda/2} (P_c)_{ik} \dot{G}_{ik} dY_3 \quad (9)$$

In this case, it is obvious that no unphysical energy source arises, as the cohesive stress \mathbf{P}_c is doing work through the deformation rate that actually produces the stress. Inserting equation (4) into this relation yields:

$$\begin{aligned} \dot{E}_{\mathcal{L}_2} &= \int_{-\lambda/2}^{\lambda/2} \left((P_c)_{ij} \dot{F}_{ij} \right) dY_3 - \bar{P}_{ij} (\dot{u}_i^+ N_j^+ + \dot{u}_i^- N_j^-) \\ \text{where } \bar{P}_{ij} &= \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} (P_c)_{ij} dY_3 \end{aligned} \quad (10)$$

Comparing (8) to (10) suggests that the cohesive traction can be defined, such that no energy source exists, as:

$$(p_c)_i^{+-} = \bar{P}_{ij} N_j^{+-} \quad (11)$$

Thus the application of the cohesive stress consists of replacing the continuum Cauchy stress with the cohesive stress defined in equation (6) within Λ , and applying the tractions defined in equation (11) to the surfaces Γ^{+-} .

3. FINITE ELEMENT METHOD IMPLEMENTATION

The Cohesive Continuum Framework outlined in the preceding section has been implemented in a time-explicit 3D finite element structural dynamics code named CCFEM. CCFEM is written in C++ and has been successfully compiled and tested using the Gnu c++ compiler, as well as the Intel c++ compiler.

The 8-noded tri-linear hexahedral solid element is used for modeling the bulk continuum. This element utilizes an enhanced strain low order formulation similar to that proposed by de Souza Neto *et al.* [20] and Rashid and Selimotic [21] when nearly incompressible material models are specified. Furthermore, the incremental kinematics method given by Rashid [22] is used to generate constitutive input from the incremental deformation gradient.

For the purposes of this work, material separation is assumed to occur across element boundaries (i.e. inter-element facets). Candidates for the rupture surface (Γ_0) are therefore limited to element boundaries, which are referred to as separation facets. A typical such facet, together with its adjacent bulk elements and the corresponding separation layer (Λ), is shown in Figure 3. Note that the separation layer is defined such that it intrudes into the surrounding bulk elements by a distance $\lambda/2$ on each side of the separation facet. It is assumed that a portion of each element surrounding the potential separation facet contains a quantity of material subject to rupture (see Figure 3). The volume Λ is integrated using 2 to 8 integration points at a distance $Y_3 = \pm\lambda/4$ from

the facet, as indicated by the solid rectangles in Figure 4. An integration point on one side of the facet is mirrored on the other side of the facet, and together these integration points are referred to as an integration couple. The points that make up an integration couple have the same Y_1 and Y_2 coordinates, while the Y_3 coordinates have opposite sign. The number and location of the integration points should mimic the integration rule used in the bulk elements. If a fully integrated element is specified, then the choice of 8 integration points (4 couples) is made. If a reduced integration rule is used, then 2 integration points (1 couple) is used.

The material state at the CCF integration points are updated under the assumption that \mathbf{G} represents the deformation gradient in Λ . Prior to the initiation of the separation process ($\Phi < \Phi_I$), the gap vector (\mathbf{v}) is equal to zero, thus \mathbf{G} is equal to the standard continuum deformation gradient. After the initiation of the separation process, the non-zero gap vector (\mathbf{v}) is calculated for each integration couple using a pair of formerly coincident points on the separation facet. This pair of points has the same Y_1 and Y_2 coordinates as the associated integration couple, but has a Y_3 coordinate equal to zero (i.e., the points initially lie on Γ). Note that the assumed relationship between Λ and the surrounding hexahedral elements imposes some limitations on the allowable configuration of the mesh. Specifically, the hex elements adjacent to the separation faces should be cuboid, and must not have thickness less than $\lambda/2$ in the Y_3 direction, as Λ is assumed to be a subset of the adjacent hex elements. A CCF formulation that is not subject to these conditions is presented by Settgast [19]. These conditions on the mesh are retained in this exposition for clarity.

Element Splitting and Node Duplication

In a standard FEM setting, the creation of a new surface along interior element boundaries requires that node duplication occur. The duplication of a node is dependent on the values of the rupture function at the CCF integration points corresponding to the facet to which the node is connected. Specifically, whenever the value of the rupture function at one or more CCF integration point exceeds the specified value for rupture initiation ($\Phi > \Phi_I$), the corresponding facet is available for

separation. Facets with $(\Phi > \Phi_l)$ are referred to as “pending facets” to signify their readiness to participate in the node duplication process. When a node is surrounded by a collection of pending facets, such that a closed path around the node is contained in these facets, the node is duplicated, and the element connectivity is modified accordingly. A *facet path* is formed by traversing facet edges to move between neighboring pending facets. A *closed path of pending facets* implies that there exists a path that leads back to the pending facet at which the path originated. This logic is illustrated in Figure 5, where one non-duplication condition is presented along with two duplication conditions. Once a closed path is found, the node is duplicated to form a new *node pair*, and element connectivity is reassigned such that one node belongs to all elements on one side of the facet path, and the other node belongs to elements on the opposite side.

Cohesive Stresses and Nodal Forces

Once nodes are duplicated, nodal force contributions corresponding to the cohesive stress must be applied to the body. The addition of a cohesive stress term requires that extra terms be added to the weak equations of motion. The extra terms mimic the application of traction to a surface, as well as the presence of a cohesive stress state in Λ . The finite element discretized equations of motion are:

$$\begin{aligned}
\sum_{k=1}^{nelem} \sum_{b=1}^{nnip} (\rho_0 a_{ai}^{n+1} |\mathbf{J}_b|) &= \sum_{m=1}^{ntbc} \sum_{b=1}^{nfip} \left\{ \left[(N_a \bar{p}_i^{n+1}) \right]_b |\mathbf{J}_b| \mathbf{J}_b^{-T} \mathbf{N} \right\} - \sum_{k=1}^{nelem} \sum_{b=1}^{nbip} \left\{ (N_{a,j} P_{ij}^{n+1}) \right]_b |\mathbf{J}_b| \right\} \\
&+ \sum_{m=1}^{ncf} \sum_{b=1}^{nccfip} \sum_{side=1}^2 \left\{ \left(N_a (-1)^{side+1} (\mathbf{p}_c^{n+1})_i \right) \right]_b |\mathbf{J}_b| \mathbf{J}_b^{-T} \mathbf{N} \right\} \\
&- \sum_{m=1}^{ncf} \sum_{b=1}^{nccfip} \sum_{side=1}^2 \left\{ \left[N_{a,j} (\mathbf{p}_c^{n+1} - \mathbf{P}^{n+1})_{ij} \right]_b |\mathbf{J}_{\Lambda b}| \right\},
\end{aligned} \tag{12}$$

where :

N = shape functions

$a = 1, 2, 3$...number of nodes

$i, j = 1, 2, 3$

$ntbc$ = number of external facets with a traction boundary conditions

$nfip$ = number of integration points per external facets

$nelem$ = number of bulk elements

$nbip$ = number of integration points per bulk element

ncf = number of active cohesive facets

$nccfip$ = number of integration points per cohesive facet

$side$ = specify which bounding element to act upon

$$\mathbf{J}_b = \frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} \bigg|_{\boldsymbol{\xi}_b} \quad \text{for the bulk element volume}$$

$$\mathbf{J}_{\Lambda b} = \frac{\partial \mathbf{X}}{\partial \boldsymbol{\xi}} \bigg|_{\boldsymbol{\xi}_b} \quad \text{for the layer volume } \Lambda$$

The last two terms in equation (12) represent the contribution of the CCF to the equations of motion. In the additional terms, the outer summation limit “ ncf ” represents the number of cohesive facets/layers that are undergoing the separation process. The inner summation loops over the number of CCF integration points on/in a facet/layer.

The first part of the cohesive term in equation (12) applies the cohesive tractions as defined in equation 11, to the surface of the separating facet in the same manner as boundary tractions are applied to an external facet. The second part of the cohesive term provides nodal force contributions from the cohesive stress (\mathbf{P}_c) minus the bulk stress (\mathbf{P}) within volume Λ . This is done for each of the two elements that surround the separating facet. If the subtraction of \mathbf{P} were not performed, the volume Λ would essentially apply nodal force contributions twice with \mathbf{P} , and \mathbf{P}_c each being used once to represent the stress in the layer. This procedure requires that the bulk material state be calculated at the CCF integration points, i.e. the material state is tracked at the CCF integration-point locations using kinematics derived from \mathbf{F} in addition to kinematics derived from \mathbf{G} .

Cohesive Damping Traction

In structural dynamics simulations, it is often desirable to introduce damping to reduce high frequency noise that may be generated by highly localized discontinuous processes. While it is demonstrated in the following section that the CCF does not require damping to attain physically meaningful results, it is still advantageous to provide a means by which to damp high frequency motions that result from discretization of the problem. For example, use of the constant-volume element formulation appears to have slightly detrimental effects on the overall stability of problems containing active CCF elements. This stability-related behavior is often extremely subtle, and often does not appear in constant-volume element analysis. However, when the instability does appear, it may be suppressed by specifying a *cohesive damping traction* ($\mathbf{p}_{\text{damping}}$), which is proportional to the rate of the gap vector. This cohesive damping traction is defined as:

$$\mathbf{p}_{\text{damping}} = \left(2\gamma_{\text{ccf}} \sqrt{\rho_0 (\lambda_{\text{Lamé}} + 2\mu)} \right) \dot{\mathbf{v}}$$

where :

γ_{ccf} is the cohesive damping coefficient (14)

$\lambda_{\text{Lamé}}$ is the elastic Lamé's constant

μ is the elastic shear modulus

$\dot{\mathbf{v}}$ is the rate of the gap vector

With the exception of γ_{ccf} , the parameters used in equation 14 are taken from the bulk material.

Values of the cohesive damping coefficient γ_{ccf} typically range from 0.01 to 0.5, although the effects of the damping on the overall solution should always be checked to ensure that they are negligible.

4. NUMERICAL RESULTS

In this section, results from a series of Cohesive Continuum Framework-enhanced finite element analyses are presented. First, a series of CCF analyses using a linear elastic constitutive relation are presented, to provide insight into the fundamental behavior of the CCF-FEA. The CCF is then used to solve more complex problems using a Gurson-type void growth model in the bulk continuum.

For simplicity, an isotropic rupture function is specified in all analyses presented in this study. The crack path is predetermined to be along a line of geometric symmetry, which is the vertical centerline of the mesh in all cases. Thus, only the nodes along the vertical ($X_2=0$) centerline of the mesh are specified as “separable,” and are the only candidates for duplication. Furthermore, only facets along this plane $\mathbf{N}=(1,0,0)$ will participate in the separation process. While the CCF allows the specification of a directional rupture function, which leads to the ability to predict crack paths, these abilities are not discussed here and will be presented in future studies.

Constitutive Relations

The first material used in this study is a brittle steel which is described by a linearly elastic constitutive relation. Specifically, a hypo-elastic constitutive relation is specified, with the full material description being given by any two of the standard elastic constants K , λ , ν , μ . (i.e. bulk modulus, Lamé constant, Poisson’s ratio, and shear modulus respectively). In the case of elasticity, the rupture function must be constructed from the Cauchy stress tensor (\mathbf{T}), along with the normal vector to the potential rupture surface, as stress is the only state variable present. Accordingly, a simple rupture function is chosen as:

$$\Phi_{rupture} = \sigma_1 (\mathbf{s}_1 \cdot \mathbf{n}),$$

where :

$$\begin{aligned} \sigma_1 &\text{ is the maximum principal stress of } \mathbf{T}, \\ \mathbf{s}_1 &\text{ is the principal direction corresponding to } \sigma_1, \\ \mathbf{n} &\text{ is the current configuration normal to } \Gamma. \end{aligned} \tag{18}$$

This rupture function has units of stress, with Φ_1 and Φ_2 representing the stresses at which rupture initiates and completes respectively. With this maximum-normal-stress rupture function specified, a simple stress reduction factor is proposed:

$$r(s) = e^{-\alpha s} - s e^{-\alpha}. \tag{20}$$

The second material considered in this study is a forged 21-6-9 steel. As this material is expected to exhibit ductile fracture through void growth and coalescence, a measure of void growth should

influence the rupture function. Here, we use the void-growth model originally proposed by Gurson [23, 24], and later modified by Needleman and Tvegaard [25]. The matrix material is characterized by J_2 flow theory with power law hardening:

$$Y = Y_0 \left[1 + \left(\frac{\epsilon_{eps}}{\epsilon_{ref}} \right)^h \right]. \quad (21)$$

Through this relation, the magnitude of the yield stress increases with increasing effective plastic strain ($\dot{\epsilon}_{eps} = \sqrt{2/3 \mathbf{D}_p : \mathbf{D}_p}$ where \mathbf{D}_p is the plastic part of the rate of deformation deviator). The modified Gurson model specifies a yield surface that exhibits softening through terms involving the void volume fraction (f) and hydrostatic pressure. We used the yield function proposed by Needleman and Tvergaard [25]:

$$\phi_{GURSON} = \left(\frac{s_{vm}}{Y} \right)^2 + 2 \cdot Q_1 \cdot f \cdot \cosh \left(\frac{3}{2} \frac{Q_2 \cdot p}{Y} \right) - [1 + (Q_1 \cdot f)^2] = 0, \quad (22)$$

where ($S_{ij} = T_{ij} - p\delta_{ij}$) is the deviatoric stress, and ($s_{vm} = \sqrt{\frac{3}{2} S_{ij} S_{ij}}$) is the von-Mises stress. Note that the void volume fraction (f) is a variable that is intended to track the volume of the voids divided by the total volume in an arbitrary region. While the existence of physical voids would introduce a length scale into the problem through the void radius or the distance between voids, the Gurson model is still a local continuum-based formulation and does not provide an actual description of finite-length features. Thus the voids are not treated as micro-structural entities. Instead, they are accounted for by considering a homogenized, unvoided material that exhibits dilatant plasticity.

The increase in void volume fraction may be attributed to the volumetric portion of the plastic strain tensor:

$$\dot{f} = (1 - f) \text{tr}(\mathbf{D}_p). \quad (23)$$

In addition to growth of existing voids, the ability to nucleate voids is essential to the modeling process. Various nucleation models have been proposed by Gurson [24], and Needleman and Rice

[26], and Chu and Needleman [27], among others. A combination of these approaches is used as follows:

$$\dot{f}_{nucleation} = \dot{\epsilon}_p \frac{f_\epsilon}{\sigma_\epsilon \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{\epsilon - \epsilon_N}{\sigma_\epsilon} \right)^2} + \dot{p}_{max} \frac{f_p}{\sigma_p \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{p_{max} - p_N}{\sigma_p} \right)^2},$$

where :

- $\dot{\epsilon}_p$ is the rate of effective plastic strain
- \dot{p}_{max} is the rate of increase in the maximum pressure seen by the material
- f_ϵ is the maximum void volume fraction nucleated by the strain term
- f_p is the maximum void volume fraction nucleated by the pressure term
- ϵ_N is the mean strain at which the distribution is centered
- p_N is the mean pressure at which the distribution is centered
- σ_ϵ is the standard deviation of strain based distribution
- σ_p is the standard deviation of pressure based distribution.

(24)

This relation specifies that the nucleation of voids is normally distributed around a mean effective plastic strain and a mean pressure. The amount of void volume fraction that may be nucleated through strain and pressure is equal to f_ϵ and f_p respectively. Note that Chu and Needleman [27] use $(p+Y)$ rather than p for the stress-based nucleation.

Since the void volume fraction provides a direct measure of the amount of voids present in a material, it is a prime candidate for use in the rupture function. In this work the non-directional rupture function is simply set equal to the void volume fraction with a directional factor similar to that used in the linear elastic material.

$$\Phi_{rupture} = f(\mathbf{s}_1 \cdot \mathbf{n}) \quad (18)$$

Table 1 presents a summary of material parameters used in the subsequent analyses. In the Gurson model, the values of Q_1 and Q_2 are taken from Tvergaard [28, 29]. Brown and Embury [30] and Andersson [31] provide guidelines for initial estimates of Φ_2 .

Material Model	Linear Elastic	Gurson

	$\rho = 7900 \text{ kg/m}^3$ $E = 1.9\text{E}11 \text{ Pa}$ $\nu = 0.3$	$\rho = 7900 \text{ kg/m}^3$ $E = 190 \text{ GPa}$ $\nu = 0.3$ $Y_0 = 6.8\text{E}8 \text{ Pa}$ $\varepsilon_{\text{ref}} = 0.58$ $h = 0.56$ $f_{\text{init}} = 0.0$ $Q_1 = 1.5$ $Q_2 = 1.0$ $f_\varepsilon = 0.02$ $\varepsilon_N = 0.3$ $\sigma_\varepsilon = 0.1$ $f_p = 0.005$ $p_N = 1750 \text{ MPa}$ $\sigma_p = 250 \text{ MPa}$
Rupture Parameters	$\Phi = \sigma_1$ $\Phi_1 = 500 \text{ MPa}$ $\Phi_2 = 2000 \text{ MPa}$	$\Phi = f$ $\Phi_1 = 0.01$ $\Phi_2 = 0.3$
Stress Reduction Function	$r(s) = e^{-\alpha s} - s e^{-\alpha}$ $\alpha = 0.15$	$r = (1 - s^{1.5})$
Length Scale	20 μm	100 μm

Table 1: Summary of Constitutive Relations

Uniaxial Behavior

To examine the uniaxial response of a CCF enabled-FEA, the plate mesh shown in Figure 6 is subjected to kinematic boundary conditions such that the nodes on the right side of the mesh ($X_I=3 \text{ mm}$) are displaced in the positive X_I direction, and the nodes on the left face of the mesh ($X_I=-3 \text{ mm}$) are displaced in the negative X_I direction at a velocity of 0.01 m/s. Results from both the brittle (linear elastic) and ductile (Gurson) materials under uniaxial strain, and plane stress conditions are presented through the CCF-generated traction-separation curves. It is important to note that the traction-separation curve derived from a CCF-enabled analysis does not provide all information pertaining to the behavior of a given simulation (e.g., there are other factors in addition to tractions that effect the equations of motion). Nonetheless, the relation between cohesive tractions and gap opening displacements do provide a point of comparison to traction-separation relations used in cohesive zone methods.

Figure 7a shows the traction-separation curve for the linear elastic material with an element size of 0.1 mm. The separation process begins with a closing traction of 500 MPa ($\Phi_1=500$ MPa), rises to a peak of approximately 1300 MPa, is unloaded to zero stress, and then reloaded until the stress decays to zero at a gap-opening distance of about 1.6 μm . The uniaxial strain and plane-stress boundary conditions yield nearly identical traction separation curves, which is a result of a rupture function equal to the maximum principal stress, and a small length scale relative to the element size. A linear unload/reload curve that passes through the origin is the expected response for all linear elastic materials, as there is no concept of permanent deformation introduced by the CCF. Note that the slope of this curve is inconsequential in relation to the courant stability limit, as the strain occurs across the layer of thickness λ . In other words, a finite deformation accompanies the case when the slope of the traction-separation curve is unbounded.

Figure 7b presents traction-separation curves resulting from the use of a Gurson void growth material model. The traction-separation curves that result from the use of the Gurson model extend over a much larger range of gap opening than that of the linear elastic material (40-140 μm gap-opening), with the plane stress case being the higher of the two. Note that the unload/reload curve drops to a non-zero gap-opening value that corresponds to zero elastic strain. Due to permanent deformations not present in an elastic material model, zero elastic strain does not equate to zero gap opening displacement.

In this series of uniaxial analyses, a CCF enabled FEA is seen to simulate material separation for both brittle and ductile materials by simply specifying different bulk constitutive models, rupture functions, and appropriate CCF parameters. The inherent ability of a CCF enabled FEA to seamlessly manage unloading/reloading within the context of the selected material model is demonstrated.

Multiaxial Cyclic Behavior

While the previous analyses illustrate the capability of the CCF enabled FEA to undergo unloading/reloading, real world problems require complete flexibility to simulate arbitrarily complex loading. To this end, the manner in which a CCF enabled FEA handles complex loading paths is explored using the plate mesh shown in Figure 6. The mesh is subjected to a loading path that combines axial/shear and loading, contains several changes in the loading directions, including a compressive cycle. The linear elastic constitutive model is used in this simulation. Figure 8 illustrates the loading path in terms of displacement vectors, which are applied to the left and right extremes of the mesh via velocity boundary conditions (note that the B.C. applied to the left extreme is the negative of the path shown). In addition, images of the deformed meshes (displacements are magnified by a factor of 100) are shown to illustrate the effects that a loading path has on the mesh. A particular portion of the loading path is identified by the letter that is placed at the end of the path in Figure 8. The magnitude of the specified velocities start at zero, increase linearly throughout the first half of the loading segment, then decrease linearly to zero at the end of the loading segment. Figure 9 plots the average normal and average shear Cauchy tractions against the average normal and average shear opening displacement within one of the facets along the separation plane. The letters on the plots are used to signify the end of each loading path as defined in Figure 8.

Loading path A is a combination of normal tension and shear. At some point during this loading, the rupture criterion is satisfied for all facets on the potential separation plane, node duplication occurs, and the separation process begins. Loading path B is a shear load that reverses the component of shear loading from path A, but keeps the normal displacement fixed. During this loading path, the shear traction and gap displacement completely reverse direction in a linear fashion, while the normal traction stays essentially constant. Loading path C is identical in direction to loading path A, but at the end of this loading path, the problem ends up in pure normal tension. As expected, the normal component of the traction and gap vectors increase in a manner similar to what is observed during loading path A. The normal component ends at some positive value, while

the shear component approaches the origin (i.e. zero shear gap-displacement, and zero shear cohesive stress). Loading path D then enforces a normal compression on the mesh. The normal components of the traction and gap vector approach zero in a linear fashion, similar to the unload/reload cycles observed in the uniaxial strain loading. Once the origin is reached and intrusion occurs, the cohesive stress reverses its sign and pushes the separation surfaces apart (i.e. the cohesive stress is no longer a closing traction). However, as long as a stress-reduction factor of less than unity is applied to the cohesive stresses, a finite amount of intrusion cannot be prevented. Attempts to set the stress reduction factor to unity while intrusion is taking place have resulted in numerical complications. (This detail will be addressed in future work.) Thus, this loading illustrates how the CCF provides resistance to intrusion naturally, but does not provide a strict no-interpenetration rule. Loading path E again mimics the loading from A and C. The normal loading curve moves back up the unload/reload curve from D, but departs from the curve when the separation coefficient begins to evolve (i.e. when the rupture function reaches its maximum value over its history). The mesh is loaded until complete separation occurs, although the final portion of the traction separation-curve is not shown for clarity.

The results of this simulation show that a CCF enabled FEA possesses a natural ability to simulate fracture problems which are subjected to combined loading, changes in loading direction, unloading/reloading, and post-separation compression.

Time Continuity

Through the previous two examples, the ability of a CCF enabled FEA to produce a time continuous solution is explored. Prior to a discussion of the simulation results, a quantitative measure by which time continuity is measured, the *net normalized nodal acceleration* ($\Delta \mathbf{a}_{nnn}$), is defined as:

$$\Delta \mathbf{a}_{nnn} = \frac{(\mathbf{f}_{cohesive} + \mathbf{f}_{bulk}) / (\frac{1}{2}m) - \mathbf{f}_{nc_bulk} / (m)}{|\mathbf{f}_{cohesive}| / (\frac{1}{2}m)} \quad (25)$$

where:

m = nodal mass prior to duplication

$\mathbf{f}_{\text{cohesive}}$ = nodal force from cohesive stresses

\mathbf{f}_{bulk} = nodal force from connected bulk elements (post-duplication)

$\mathbf{f}_{\text{nc_bulk}}$ = nodal force from connected bulk elements (pre-duplication)

For a perfectly time continuous method, $\Delta \mathbf{a}_{\text{nnn}}$ should equal zero immediately after separation, thus deviation from zero represents a time discontinuity. In the case of uniaxial loading, the CCF displays excellent time continuity characteristics as $|\Delta \mathbf{a}_{\text{nnn}}| < 10^{-8}$, which is essentially zero in this numerical setting. However in the case of multi-axial loading such as in loading path A in the preceding example, the values of $\Delta \mathbf{a}_{\text{nnn}}$ are not zero. Table 2 summarizes $\Delta \mathbf{a}_{\text{nnn}}$ for each duplicated node when combined axial-shear loading is applied.

Node	$\Delta \mathbf{a}_{\text{nnn}}$ (X_1 -direction)	$\Delta \mathbf{a}_{\text{nnn}}$ (X_2 -direction)	$\Delta \mathbf{a}_{\text{nnn}}$ (X_3 -direction)
1 (Edge)	-0.0400	-0.0185	-0.0446
2	0.0022	0.0136	-0.0298
3	0.0142	0.0028	-0.0124
4 (Middle)	0.0211	0.0109	0.0000

Table 2

Because the nodal contributions from the formerly connected bulk elements are replaced by the nodal contributions from the cohesive tractions instantaneously, any difference in these values results in a non-physical impulse loading. Note that the cohesive tractions fully describe the effects of the cohesive stress at the time of separation, as the bulk state is equal to the cohesive state, leading to a nodal force contribution of zero inside Λ . From the results presented in Table 2, it is apparent that this CCF implementation does not guarantee time continuity for all meshes and loading directions. The logical remedy to this situation is to apply a nodal force scaling in

conjunction with the contributions from the cohesive tractions to enforce time-continuity. However, such options are not explored here.

Brittle Fracture of a Double Cantilever Beam Specimen

In this section, the brittle fracture of a double cantilever beam specimen is simulated. The first result presented is a mesh refinement study on four linearly elastic DCB meshes. The four levels of refinement and their corresponding minimum smallest element size are Coarse (0.4 mm), Medium (0.2 mm), Fine (0.1 mm), and Very Fine (0.05 mm). Mesh refinement is confined to the regions near the predetermined rupture surface, as illustrated in Figure 10. The DCB meshes are subjected to a normal (Mode I) opening velocity of 50 mm/s (increasing linearly from zero over 0.01 s). These simulations were run until approximately 20 mm of crack growth was achieved.

The results of these analyses are presented as plots of the *opening force vs crack mouth opening displacement (CMOD)* and *Rate of Energy Dissipation (i.e. G) vs Crack Extension*. The *opening force* and *CMOD* are readily available as output from the finite element code, while the rate of energy dissipation is calculated by taking the total energy dissipated over a period of time, and dividing it by the amount of new surface area created over that period of time. Thus, the rate of energy dissipation at any time t is expressed as:

$$G(t) = \frac{EnergyDissipated(t + \Delta t) - EnergyDissipated(t - \Delta t)}{SurfaceArea(t + \Delta t) - SurfaceArea(t - \Delta t)}, \quad (26)$$

where Δt is some increment in time. The dissipated energy is calculated by subtracting the kinetic and elastic strain energies from the total energy input to the system. The surface area is calculated by summing the area of all CCF facets multiplied by their separation coefficients. Thus an unruptured ($s=0$) facet will contribute zero area, and a fully ruptured ($s=1$) facet will contribute all of its area to the summation. Note that if very small values of Δt are used in Equation (26), then the

discrete nature of the numerical solution introduces the possibility of a divide-by-zero situation. In order to attain physically meaningful results, a value of $\Delta t = 100 \mu s$ is used here.

Figure 11 plots the rate of energy dissipation vs crack extension for the four levels of refinement. The dissipation rates are centered about a constant value ($\sim 765 \text{ J/m}^2$) throughout the extension process, which is expected considering the double-cantilever geometry. The data indicates that the solution has essentially converged for the “fine” and “very fine” levels of refinement, with the “coarse” and “medium” levels of refinement oscillating around the converged solution. Figure 12 plots the *Force* vs *CMOD* for the various levels of mesh refinement. In order to smooth the force-time history, a 4th order low-pass Butterworth filter with a cutoff frequency of 10,000 Hz was applied. The force data exhibit large oscillations that decrease as the mesh is refined. This results from a combination of smaller facet areas (smaller loss of cohesive force per facet), and a more finely discretized rupture zone (smoother temporal transition to full separation for a given facet). Since a linear elastic material is specified, LEFM along with elementary beam-theory is used to determine the force (P) and displacement ($CMOD$) given the energy dissipation rate (G) and crack size (a). This LEFM solution is plotted in Figure 12 as the heavy dotted black line, and it is confirmed that the simulation data are consistent with the theoretical LEFM solution. As is the case in Figure 11, Figure 12 also indicates that the “fine” and “very fine” meshes have converged to a satisfactory level.

The Cohesive Continuum Framework’s ability to model multi-mode fracture is demonstrated through simulations involving the “fine” mesh individually subjected to mode I (normal opening), mode II (in-plane shear), mode III (out-of-plane shear), and multi-mode (I, II, and III) loading. This mesh, which is shown in Figure 10, consists of 89,967 nodes, 6817 separable nodes, and 83,200 elements. To attain the various loadings, nodes at the end of the double-beam are subjected to velocity boundary conditions. Specifically, the individual mode I, II, and III loadings are produced by specifying the velocity of the nodes on one face in one direction, and the nodes on the other face

in the opposite direction. Thus the free ends of the beams are allowed to rotate as well as displace. For the multi-mode loading, these nodes are subject to specified velocities in all directions, and the ends of the beam translate with no rotation.

Figure 13 provides a plot of *Energy Dissipation Rate vs Crack Extension*. The mode I loading case produces a result equivalent to the mesh refinement study with an energy dissipation rate of approximately 765 J/m^2 . The two shear modes (II and III) exhibit dissipation rates that are nearly equivalent to each other, except for a slight deviation of the mode II case near the end of the crack extension. This is due to beam bending in the mode II loading, which adds a mode I component to the crack tip loading state. The difference in dissipation rates between the shear cases and the normal case is a result of how the normal and shear components of stress evolve differently in the constitutive relation. Furthermore, the choice of rupture function (Φ) is specified to be equal to the maximum principal stress, and thus the rupture function evolves differently for the two cases.

Simulation of a 3-Point Bend Specimen

In this section, experimental data from three separate 3-point bend specimens of 21-6-9 steel are compared with a CCF simulation. The 3-point bend test involves pre-cracking the specimen at mid-span, then applying a velocity at mid-span while the specimen is simply supported. The meshed 3-point bend specimen is illustrated in Figure 14, along with relevant dimensions. Note that the side view in Figure 14 is of a deformed mesh, although the dimensions refer to the un-deformed geometry. The mesh is refined near mid-span, and consists of 26,783 nodes and 23,820 elements with a minimum element dimension of 0.006 mm. A pre-crack of length 2.58 mm, which runs through half the specimen height, is specified by duplicating nodes up the centerline. At the left and right extremes of the mesh, a set of nodes (4 nodes high and through the thickness of the beam = 42 nodes) is given a fixed kinematic boundary condition in the vertical direction. A set of nodes (6 nodes wide and through the thickness of the beam = 273 nodes) along the top mid-span surface of

the beam is then subjected to a velocity boundary condition in the negative vertical direction of 0.05 m/s.

Figure 15 provides a cut-away view of the separation plane near the conclusion of the test, with the active facets colored according to the current value of the separation coefficient. The color scheme is such that red indicates near full separation ($s=1$) and blue indicates minimal separation. Note that there are about 4 facets undergoing the separation process along the general direction of crack propagation, which suggests sufficient resolution based on mesh refinement studies. The crack front leads slightly at the edges (concave up) due to the presence of the side-notches, which create a stress state similar to plane strain throughout the width of the specimen, as well as producing a stress concentration near the outer surface of the specimen. This behavior is confirmed by images of the physical specimen (not shown), in which the specimen was cut along the separation plane after testing to reveal the shape of the rupture front.

Figure 16 shows a plot of the *applied top force* vs *CMOD* for both the simulation and experiment. Note that the experimental data is produced from three specimens that were taken from different locations in a rolled billet, thus substantial variation in material properties is expected. When viewing these results, it is important to note that the constitutive parameters were taken from a separate uniaxial tension test, while the rupture parameters used in the simulation were calibrated to provide response that is consistent with an average of the experimental data. Thus this is not a “blind” prediction but rather a demonstration that the CCF together with the Gurson dilatant plasticity model is capable of modeling ductile rupture through void growth and coalescence in a 21-6-9 steel.

In addition to the full 3-dimensional geometry, a 3-point bend sheet mesh was also studied. This sheet mesh is similar to the previous geometry in plane, but only 1 mm through the thickness of the specimen. This mesh consists of 6459 nodes and 4612 elements with a minimum element dimension of 0.006 mm. A pair of constraints in the through-thickness direction is used to

approximate plane stress or plane strain. The plane stress condition is achieved by simply constraining a single face of the specimen in the through-thickness direction, while the plane strain constraint is a result of confining both front and back surfaces in the through-thickness direction. Figure 17 shows the force per unit thickness against the *CMOD* for both the plane stress and plane strain analyses. As would be expected, the plane stress condition is observed to be much “tougher” than the plane strain condition, retaining its load carrying capacity well past the point at which the plane strain case has lost capacity.

Figure 18 shows the total energy dissipation rate (energy per separated area) against crack extension for all 3-point bend simulations. This figure shows that the plane strain case is similar to the fully 3-dimensional simulation, while the plane stress problem dissipates approximately ten times more energy than the others. This trend is expected due to greater plastic dissipation in the bulk material in the plane-stress case addition to the higher levels of dissipation associated with the surface generation as specified by the CCF.

5. Summary and Direction of Future Work

The Cohesive Continuum Framework (CCF) has been presented as a new tool for modeling the material separation in a continuum body. While the CCF draws motivation from current cohesive zone methodology presented in, e.g., [3-14], it is the goal the CCF to address certain shortcomings of standard cohesive zone formulations. In particular, the lack of an intrinsic dependence on near-tip constraint level is of substantial concern as discussed in [15-18]. Other issues include the mesh dependence of initially elastic cohesive zone models [13], and the initialization and time continuity of initially rigid cohesive zone models [14].

The CCF postulates that a standard bulk constitutive relation has the capability to generate cohesive stresses if appropriate kinematic input can be provided. From this postulate, the concept of the gradient-like tensor \mathbf{G} is introduced. The CCF formulation presented in this study assumes the

rupture process occurs within a finite layer of thickness λ of material in which \mathbf{G} is an appropriate measure of deformation for the purposes of a constitutive update. Through \mathbf{G} , deformations from the surrounding bulk are combined with the gap vector and a length scale to generate kinematical quantities, which are then used to update a material state through the bulk constitutive relation. This material state is in turn utilized to generate a cohesive stress that is applied within the rupture zone. To quantify the progression towards material rupture, a scalar rupture function (Φ) is defined from the material state in the rupturing layer. Thus, the material model is required to supply state variables that may be used to correlate and quantify the progression toward rupture. Critical values of the rupture function specify when the material separation process begins (Φ_1), and when the process is completed (Φ_2).

Issues pertaining to the implementation of the CCF in a 3-dimensional structural dynamics finite element code have been discussed. Through use of this code, it has been shown that the CCF-enabled FEA is capable of modeling the rupture process through complex loading paths (i.e. change in loading direction, unloading, compression). Through simulations of a double cantilever beam, the CCF-enabled FEA is shown to seamlessly integrate combinations of mode I, mode II, and mode III loading cases. Simulation of the ductile fracture of a 3-point bend specimen is presented, and good agreement with experiment is achieved. Finally the ability of the CCF-enabled FEA to naturally account for confinement at the crack tip has been demonstrated.

It has been demonstrated that the Cohesive Continuum Framework offers some attractive capabilities that are absent from the standard cohesive zone construct. However, outstanding issues such as element size/shape constraints, time continuity require further development. Also of practical importance is revising the implementation presented here, such that computational costs are reduced.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

References

1. D.S. Dugdale, "Yielding of steel sheets containing slits", *Journal of the Mechanics and Physics of Solids*, Vol. 8, pp. 100-104, (1960).
2. G.I. Barenblatt, "The mathematical theory of equilibrium cracks in brittle fracture", *Advances in Applied Mechanics*, Vol. 7, pp. 55-129, (1962).
3. A. Needleman, "A continuum model for void nucleation by inclusion debonding", *Journal of Applied Mechanics*, Vol. 54, pp. 525-531, (1987).
4. A. Needleman, "An analysis of decohesion along an imperfect interface", *International Journal of Fracture*, Vol. 42, pp. 21-40, (1990).
5. J. R. Rice and J.S. Wang, "Embrittlement of Interfaces by Solute Segregation", *Materials Science and Engineering*, Vol. A107, pp. 23-40, (1989).
6. X.P. Xu and A. Needleman, "Numerical simulations of fast crack growth in brittle solids", *J. Mech. Phys. Solids*, Vol. 42, pp. 1397-1434, (1994).
7. X.P. Xu and A. Needleman, "Numerical simulations of dynamic interfacial crack growth allowing for crack growth away from the bond line", *Int. J. Fracture*, Vol. 74-3, pp. 253-275, (1995).
8. X.P. Xu and A. Needleman, "Numerical simulations of dynamic crack growth along interface", *Int. J. Fracture*, Vol. 74-4, pp. 289-324, (1995).
9. V. Tvergaard and J.W. Hutchinson, *Journal of the Mechanics and Physics of Solids*, Vol. 40, pp. 1377-1397, (1992).
10. G.T. Camacho and M. Ortiz, "Computational Modelling of Impact Damage in Brittle Materials", *Int. J. Solids Structures*, Vol. 33, pp. 2899-2938, (1996).
11. G.T. Camacho and M. Ortiz, "Adaptive Lagrangian modelling of ballistic penetration of metallic targets", *Comp. Methods Appl. Mech. Engrg.*, Vol. 142, pp. 269-301, (1997).
12. M. Ortiz and A. Pandolfi, "Finite-deformation irreversible cohesive elements for three-dimensional crack-propagation analysis", *International Journal of Numerical Methods in Engineering*, Vol. 44, pp. 1267-1282, (1999).
13. P. Klein, J. Foulk, E.P. Chen, S. Wimmer, H. Gao, "Physics based modeling of brittle fracture: cohesive formulations and applications and mesh-free methods", *Sandia National Laboratory Technical Report*, SAND2001-8099, (2000).
14. K.D. Papoulia, Chin-Hang Sam, and S.A. Vavasis, "Time Continuity in Cohesive Finite Element Modeling", *International Journal of Numerical Methods in Engineering*, Vol. 58, pp. 679-701, (2003).
15. K.K. Mathur, A. Needleman, V. Tvergaard, "Three dimensional analysis of dynamic ductile crack growth in a thin plate", *J. Mech. Phys. Solids*, Vol. 44, pp. 439-464 (1996).
16. F. Costanzo, "A continuum theory of cohesive zone models: deformation and constitutive equations", *International Journal of Engineering Science*, Vol. 36, pp. 1763-1792, (1998).
17. T. Siegmund and W. Brocks, "Prediction of the work of separation and the implications to modeling", *Int. J. Fracture*, Vol. 99, pp. 97-116, (1999).
18. T. Siegmund and W. Brocks, "A numerical study on the correlation between the work of separation and the dissipation rate in ductile fracture", *Eng. Fracture Mech.*, Vol. 67, pp. 139-154, (2000).
19. R.R. Settigast, "Numerical Modeling of 3-Dimensional Surface Separation", Ph.D. Dissertation (2006).
20. E.A. de Souza Neto, D. Peric, M. Dutko, and D.R.J. Owen, "Design of Simple Low Order Finite Elements for Large Strain Analysis of Nearly Incompressible Solids", *International Journal of Solids and Structures*, Vol. 33, pp. 3277-96. (1996)
21. M.M. Rashid and M. Selimotic, "A three dimensional finite element method with arbitrary polyhedral elements", *International Journal of Numerical Methods in Engineering*, in press.
22. M. M. Rashid, "Incremental kinematics for finite element applications", *International Journal for Numerical Methods in Engineering*, Vol. 36, pp. 3937-3956, (1993).

23. A.L. Gurson, "Continuum theory of ductile rupture by void growth: part I—yield criteria and flow rules for porous ductile media," *ASME J. Eng. Mater. Technol.*, Vol. 99, pp. 2, (1977).
24. A.L. Gurson, "Porous rigid-plastic material containing rigid inclusions - Yield function, plastic potential, and void nucleation", *Proc. Int. Conf. Fracture*, Vol. 2A, pp 357-364, (1977).
25. A. Needleman and V. Tvergaard, "An Analysis of ductile rupture in notched bars", *J. Mech. Phys. Solids*, Vol. 32, pp. 461-490, (1984).
26. A. Needleman, and J.R. Rice, "Limits to ductility set by plastic flow localization", *Mechanics of Sheet Metal Forming*, pp. 237-267, (1978).
27. C.C. Chu and A. Needleman, "Void Nucleation effects in biaxially stretched sheets", *J. Eng. Materials Technol.*, Vol. 102, pp. 249-256 (1980).
28. V. Tvergaard, "Influence of voids on shear band instabilities under plane strain conditions." *Int. J. Fracture*, Vol. 17, pp. 389-407, (1981).
29. V. Tvergaard, "On localization in ductile materials containing spherical voids", *Int. J. Fracture*, Vol. 18, pp. 237-252, (1982).
30. L.M. Brown, Embury, J.D, "The initiation and growth of voids as second phase particles", *Proc. 3rd Int. Conf. on Strength of Metals and Alloys*, pp. 164-169, (1973).
31. H. Andersson, "Analysis of a model for void growth and coalescence ahead of a moving crack tip", *J. Mech. Phys. Solids*, Vol. 25, pp. 217-233, (1977).
32. ASTM E 1820-99. *Annual Book of ASTM Standards*, Vol. 03.01, pp. 972-1005, (1999).
33. J Oliver, AE Huespe, MFG Pulido, E Chaves, "From continuum mechanics to fracture mechanics: the strong discontinuity approach," *Eng. Fracture Mech.* 69, pp. 113-126, 2002.
34. J Oliver, AE Huespe, "Theoretical and computational issues in modelling material failure in strong discontinuity scenarios," *Comp. Meth. Appl. Mech. Eng.* 193, pp. 2987-3014, 2004.